



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:11 AM UTC

PDB ID : 8HW9 / pdb_00008hw9
BMRB ID : 36535
Title : Solution structure of ubiquitin-like domain (UBL) of human ZFAND1
Authors : Lai, C.H.; Ko, K.T.; Fan, P.J.; Yu, T.A.; Chang, C.F.; Hsu, S.T.D.
Deposited on : 2022-12-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

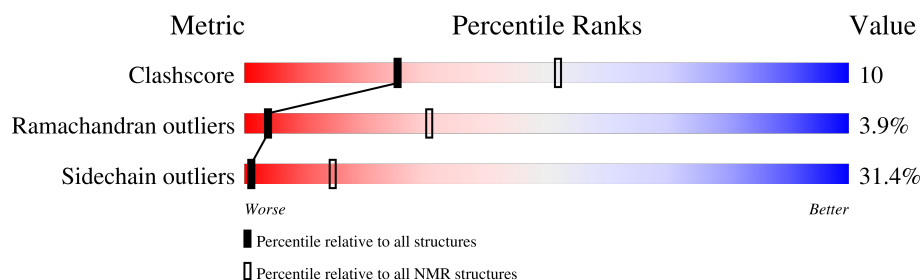
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	139	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:135-A:268 (134)	1.53	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 10, 11, 12, 14, 15, 16, 18, 20
2	2, 3, 9, 13
Single-model clusters	17; 19

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2197 atoms, of which 1098 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AN1-type zinc finger protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	139	Total	C	H	N	O	S	0
			2197	699	1098	188	205	7	

There are 3 discrepancies between the modelled and reference sequences:

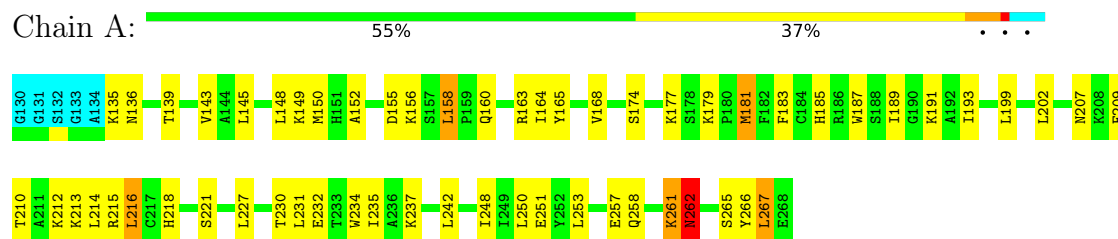
Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	-	expression tag	UNP Q8TCF1
A	131	GLY	-	expression tag	UNP Q8TCF1
A	132	SER	-	expression tag	UNP Q8TCF1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: AN1-type zinc finger protein 1

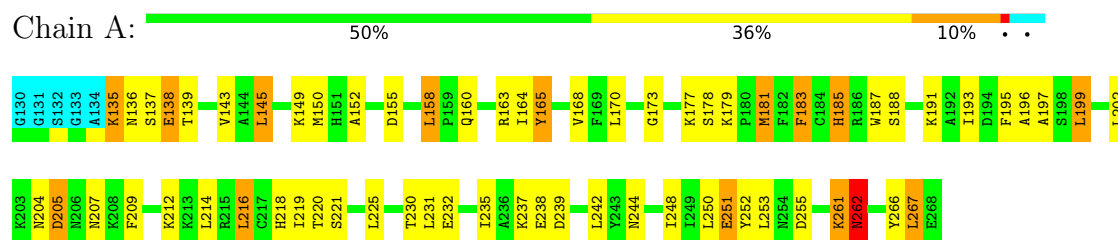


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

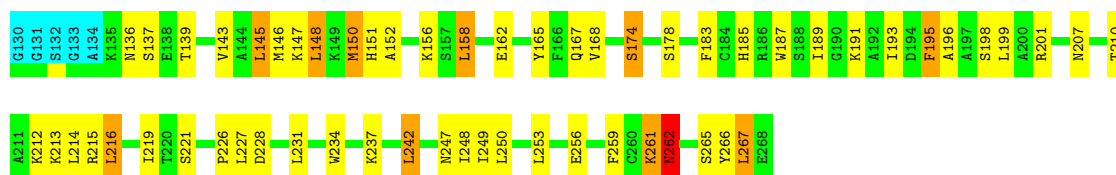
- Molecule 1: AN1-type zinc finger protein 1



4.2.2 Score per residue for model 2

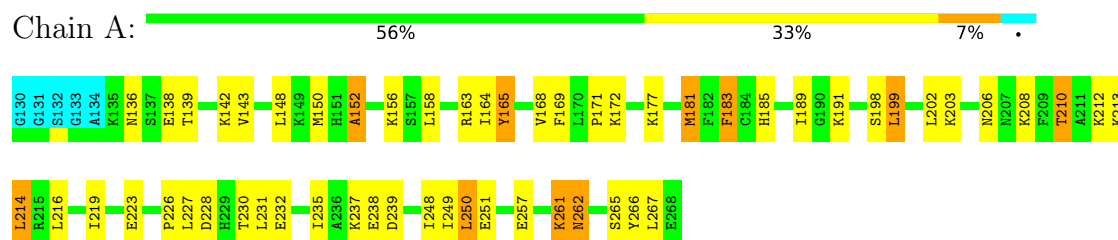
- Molecule 1: AN1-type zinc finger protein 1





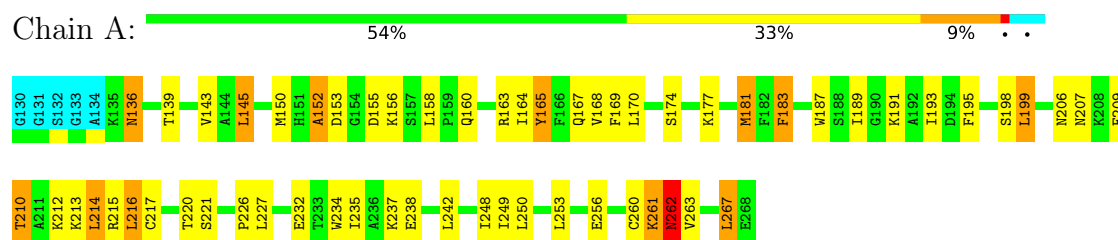
4.2.3 Score per residue for model 3

- Molecule 1: AN1-type zinc finger protein 1



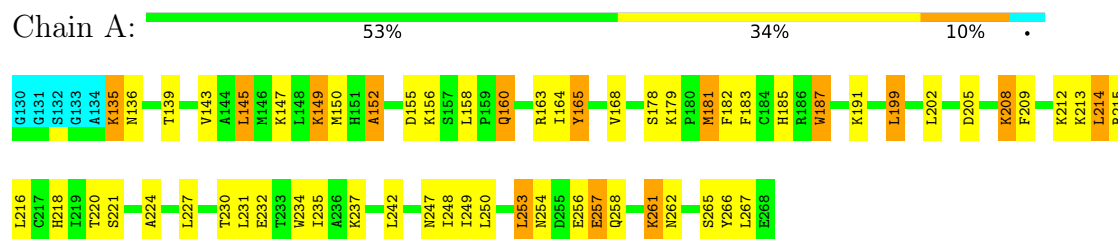
4.2.4 Score per residue for model 4

- Molecule 1: AN1-type zinc finger protein 1



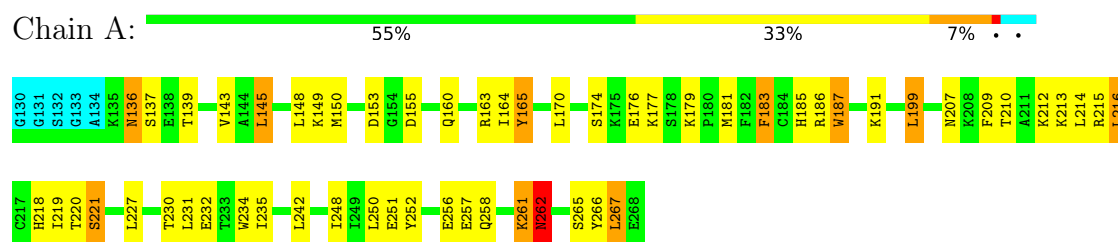
4.2.5 Score per residue for model 5

- Molecule 1: AN1-type zinc finger protein 1



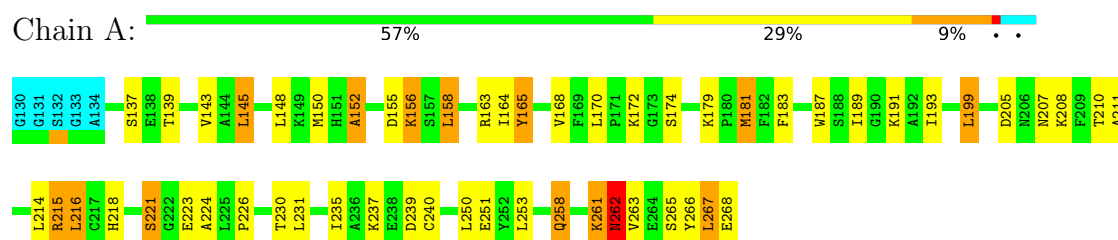
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: AN1-type zinc finger protein 1



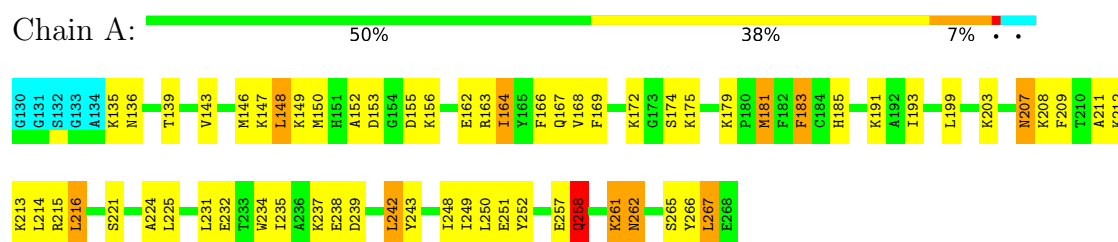
4.2.7 Score per residue for model 7

- Molecule 1: AN1-type zinc finger protein 1



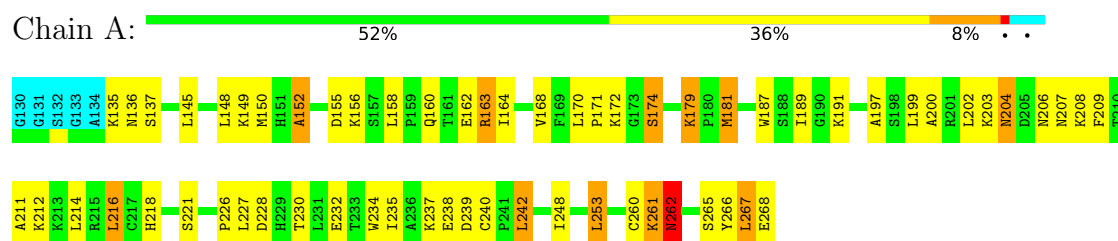
4.2.8 Score per residue for model 8

- Molecule 1: AN1-type zinc finger protein 1



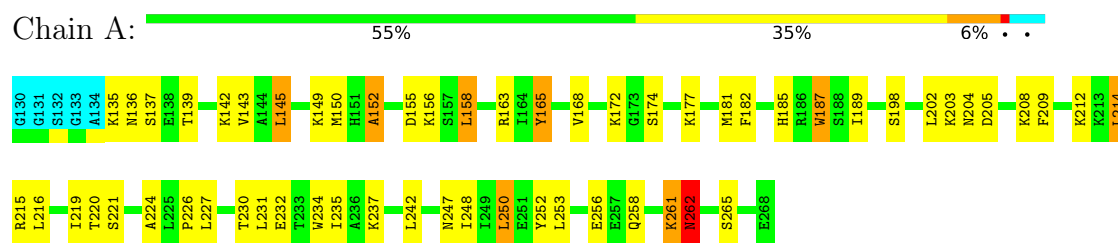
4.2.9 Score per residue for model 9

- Molecule 1: AN1-type zinc finger protein 1



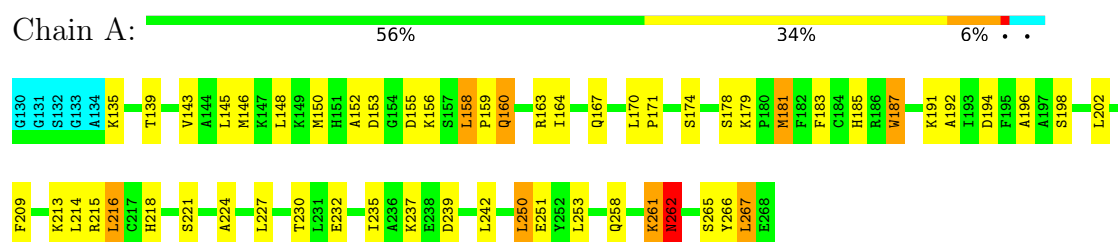
4.2.10 Score per residue for model 10

- Molecule 1: AN1-type zinc finger protein 1



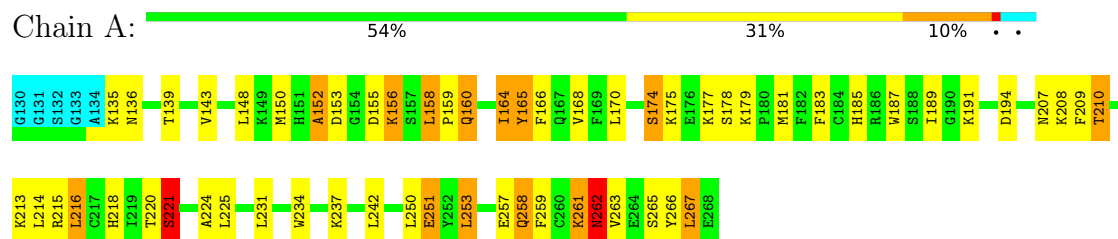
4.2.11 Score per residue for model 11

- Molecule 1: AN1-type zinc finger protein 1



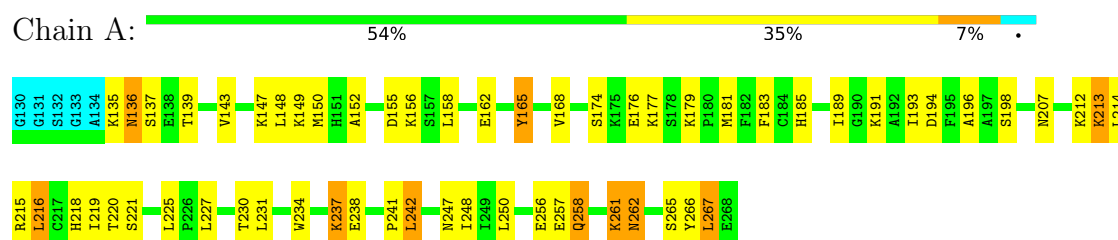
4.2.12 Score per residue for model 12

- Molecule 1: AN1-type zinc finger protein 1



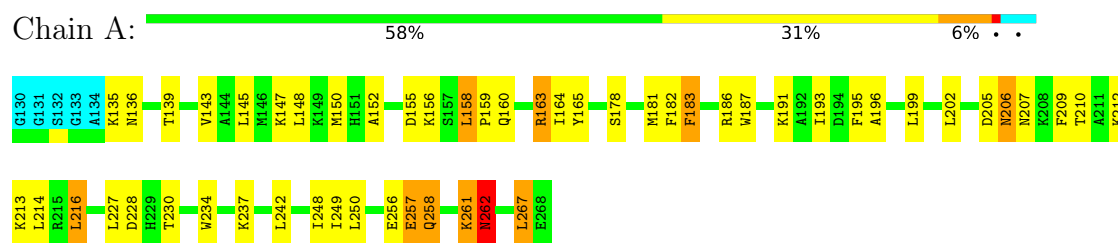
4.2.13 Score per residue for model 13

- Molecule 1: AN1-type zinc finger protein 1



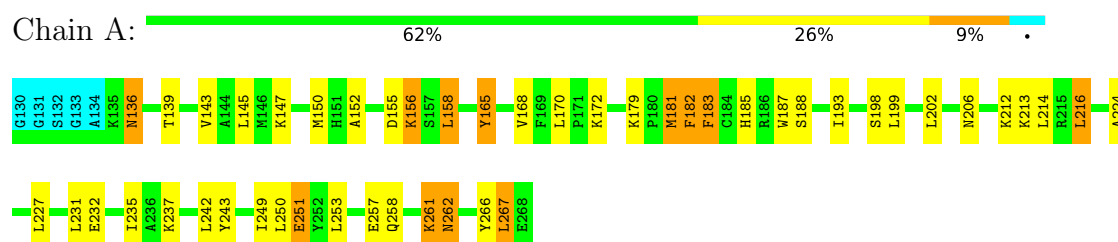
4.2.14 Score per residue for model 14

- Molecule 1: AN1-type zinc finger protein 1



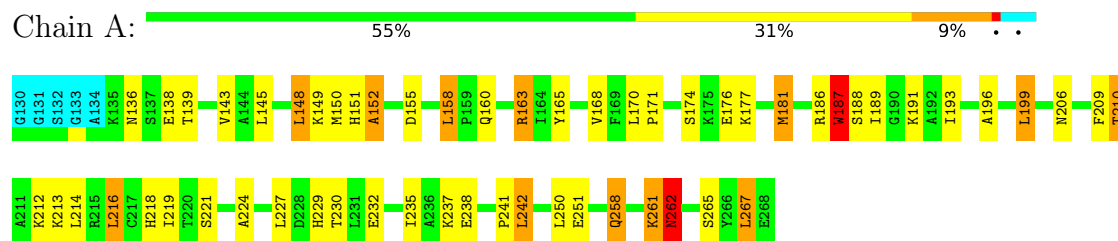
4.2.15 Score per residue for model 15

- Molecule 1: AN1-type zinc finger protein 1



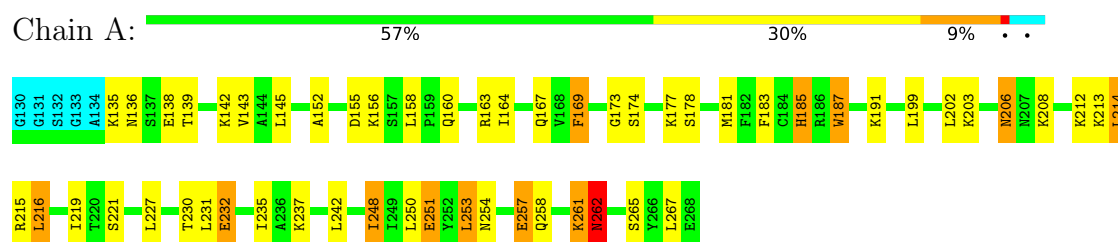
4.2.16 Score per residue for model 16

- Molecule 1: AN1-type zinc finger protein 1



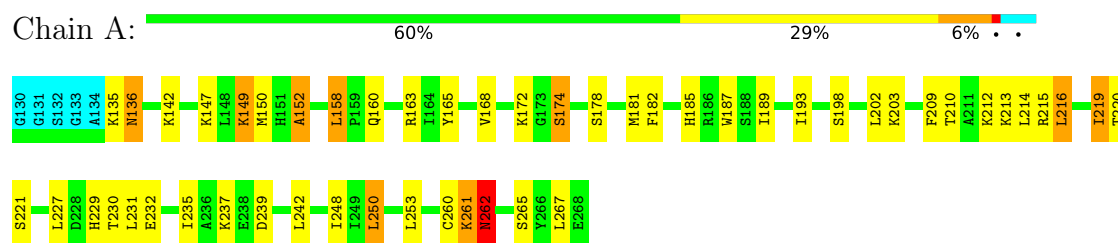
4.2.17 Score per residue for model 17

- Molecule 1: AN1-type zinc finger protein 1



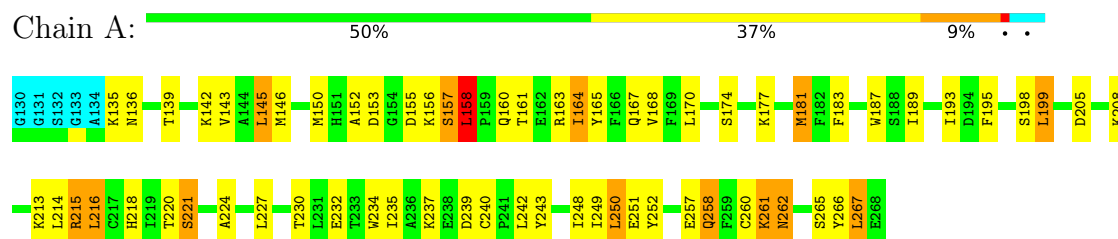
4.2.18 Score per residue for model 18

- Molecule 1: AN1-type zinc finger protein 1



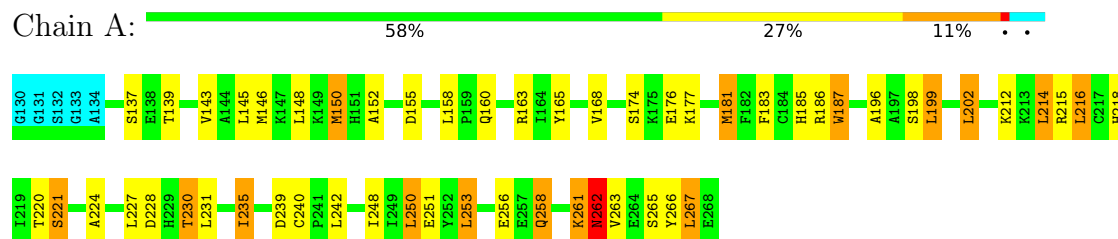
4.2.19 Score per residue for model 19

- Molecule 1: AN1-type zinc finger protein 1



4.2.20 Score per residue for model 20

- Molecule 1: AN1-type zinc finger protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.98.13

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1558
Number of shifts mapped to atoms	1558
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1076	1079	1079	22±5
All	All	21520	21580	21580	448

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:MET:HE2	1:A:150:MET:HE2	0.98	1.35	2	2
1:A:181:MET:HE2	1:A:199:LEU:HD13	0.95	1.37	15	1
1:A:181:MET:HE2	1:A:199:LEU:HD22	0.94	1.39	16	1
1:A:214:LEU:HD23	1:A:250:LEU:HD22	0.90	1.44	5	1
1:A:202:LEU:HD22	1:A:214:LEU:HD13	0.87	1.47	20	1
1:A:189:ILE:HG23	1:A:216:LEU:HD11	0.83	1.48	12	8
1:A:249:ILE:HG23	1:A:267:LEU:HD12	0.81	1.50	2	4
1:A:216:LEU:HD13	1:A:216:LEU:N	0.80	1.92	1	5
1:A:158:LEU:HD13	1:A:158:LEU:H	0.76	1.38	18	5
1:A:196:ALA:HB1	1:A:250:LEU:HD11	0.75	1.56	13	4
1:A:225:LEU:HD13	1:A:231:LEU:HD21	0.73	1.59	8	1
1:A:216:LEU:HD12	1:A:225:LEU:HD22	0.72	1.60	13	1
1:A:266:TYR:CE2	1:A:267:LEU:HD13	0.69	2.22	9	1
1:A:168:VAL:HG13	1:A:250:LEU:HD12	0.68	1.65	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:VAL:HG13	1:A:250:LEU:HD23	0.68	1.65	20	2
1:A:202:LEU:HD12	1:A:214:LEU:HD22	0.67	1.66	1	1
1:A:158:LEU:C	1:A:158:LEU:HD22	0.67	2.14	11	1
1:A:185:HIS:O	1:A:231:LEU:HD12	0.66	1.90	20	9
1:A:216:LEU:HB2	1:A:248:ILE:HD11	0.66	1.67	1	6
1:A:145:LEU:HD11	1:A:165:TYR:CZ	0.66	2.26	5	1
1:A:266:TYR:CE2	1:A:267:LEU:HD23	0.66	2.26	8	4
1:A:266:TYR:CE2	1:A:267:LEU:HD12	0.65	2.26	1	3
1:A:183:PHE:CE1	1:A:199:LEU:HD12	0.65	2.26	15	2
1:A:164:ILE:HG22	1:A:183:PHE:O	0.64	1.93	19	8
1:A:168:VAL:CG1	1:A:250:LEU:HD12	0.64	2.23	13	9
1:A:170:LEU:HD21	1:A:200:ALA:HA	0.62	1.71	9	1
1:A:216:LEU:H	1:A:216:LEU:HD22	0.62	1.54	1	1
1:A:235:ILE:HG23	1:A:242:LEU:O	0.62	1.94	16	8
1:A:216:LEU:H	1:A:216:LEU:HD13	0.62	1.53	6	2
1:A:181:MET:HG2	1:A:199:LEU:HD21	0.61	1.72	6	1
1:A:216:LEU:HD12	1:A:225:LEU:CD2	0.61	2.24	13	2
1:A:195:PHE:CZ	1:A:199:LEU:HD12	0.61	2.30	1	1
1:A:152:ALA:HB1	1:A:181:MET:HA	0.61	1.71	4	10
1:A:145:LEU:HD11	1:A:165:TYR:CE1	0.61	2.31	14	4
1:A:145:LEU:HD13	1:A:165:TYR:CE2	0.61	2.31	1	1
1:A:145:LEU:HD21	1:A:158:LEU:CD2	0.61	2.25	2	1
1:A:185:HIS:O	1:A:231:LEU:HD13	0.61	1.96	5	3
1:A:185:HIS:C	1:A:231:LEU:HD13	0.61	2.19	15	1
1:A:169:PHE:CD2	1:A:249:ILE:HD13	0.60	2.31	3	1
1:A:189:ILE:HG23	1:A:216:LEU:CD1	0.60	2.24	12	3
1:A:152:ALA:HB2	1:A:182:PHE:CE2	0.60	2.31	10	2
1:A:249:ILE:HG23	1:A:267:LEU:CD1	0.60	2.26	2	1
1:A:187:TRP:O	1:A:231:LEU:HD12	0.60	1.96	15	3
1:A:234:TRP:HB3	1:A:242:LEU:HD21	0.59	1.75	4	10
1:A:170:LEU:HD22	1:A:179:LYS:HE2	0.59	1.74	9	1
1:A:157:SER:C	1:A:158:LEU:HD22	0.59	2.22	19	1
1:A:158:LEU:HD22	1:A:158:LEU:O	0.58	1.99	11	2
1:A:139:THR:O	1:A:143:VAL:HG23	0.58	1.99	4	18
1:A:170:LEU:HD11	1:A:179:LYS:CG	0.58	2.29	7	1
1:A:181:MET:CB	1:A:199:LEU:HD11	0.58	2.28	1	1
1:A:215:ARG:O	1:A:250:LEU:HD13	0.58	1.97	19	3
1:A:219:ILE:HG13	1:A:220:THR:HG23	0.57	1.75	1	1
1:A:158:LEU:HD13	1:A:165:TYR:OH	0.57	1.99	13	2
1:A:193:ILE:HD13	1:A:216:LEU:CD2	0.57	2.28	15	2
1:A:202:LEU:CD1	1:A:214:LEU:HD22	0.57	2.28	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:231:LEU:O	1:A:235:ILE:HD12	0.57	2.00	7	1
1:A:169:PHE:CD1	1:A:249:ILE:HD13	0.57	2.35	8	1
1:A:170:LEU:HD11	1:A:179:LYS:HG2	0.57	1.75	7	2
1:A:253:LEU:HD12	1:A:266:TYR:CZ	0.57	2.35	5	1
1:A:158:LEU:HD13	1:A:158:LEU:N	0.56	2.15	1	2
1:A:225:LEU:CD1	1:A:231:LEU:HD21	0.56	2.28	8	1
1:A:215:ARG:C	1:A:250:LEU:HD13	0.55	2.26	6	1
1:A:156:LYS:O	1:A:158:LEU:HD13	0.55	2.00	12	2
1:A:148:LEU:HD13	1:A:151:HIS:NE2	0.55	2.16	2	2
1:A:181:MET:HG2	1:A:199:LEU:HD11	0.55	1.78	14	1
1:A:216:LEU:N	1:A:216:LEU:CD1	0.55	2.64	1	1
1:A:216:LEU:CB	1:A:248:ILE:HD11	0.55	2.32	1	1
1:A:145:LEU:HD11	1:A:158:LEU:HD21	0.55	1.79	9	1
1:A:253:LEU:HD23	1:A:257:GLU:HG3	0.55	1.79	17	1
1:A:170:LEU:HD22	1:A:179:LYS:CE	0.54	2.32	9	1
1:A:240:CYS:O	1:A:242:LEU:HD23	0.54	2.02	9	1
1:A:158:LEU:HD12	1:A:182:PHE:CD1	0.54	2.38	5	1
1:A:216:LEU:HD13	1:A:216:LEU:H	0.54	1.63	20	2
1:A:181:MET:HE2	1:A:199:LEU:CD2	0.54	2.26	16	1
1:A:219:ILE:HG21	1:A:247:ASN:OD1	0.54	2.01	10	3
1:A:158:LEU:HD23	1:A:163:ARG:HD3	0.54	1.79	9	1
1:A:214:LEU:HD23	1:A:250:LEU:HD12	0.54	1.78	18	1
1:A:221:SER:N	1:A:263:VAL:HG11	0.53	2.17	20	2
1:A:215:ARG:NH1	1:A:224:ALA:HB1	0.53	2.18	10	1
1:A:215:ARG:C	1:A:250:LEU:HD23	0.53	2.27	7	1
1:A:145:LEU:HD11	1:A:165:TYR:OH	0.53	2.03	10	3
1:A:152:ALA:HB3	1:A:182:PHE:CE1	0.53	2.38	15	1
1:A:215:ARG:O	1:A:250:LEU:HD23	0.53	2.02	11	3
1:A:170:LEU:HD12	1:A:179:LYS:CD	0.53	2.33	11	1
1:A:145:LEU:HD13	1:A:165:TYR:OH	0.53	2.03	15	1
1:A:214:LEU:CD2	1:A:250:LEU:HD12	0.53	2.33	18	1
1:A:193:ILE:HG23	1:A:214:LEU:O	0.53	2.03	1	3
1:A:202:LEU:HD13	1:A:252:TYR:OH	0.53	2.04	1	1
1:A:224:ALA:HB3	1:A:258:GLN:O	0.53	2.04	15	9
1:A:266:TYR:CD2	1:A:267:LEU:HD23	0.52	2.39	8	4
1:A:232:GLU:HA	1:A:235:ILE:HD12	0.52	1.81	16	13
1:A:241:PRO:C	1:A:242:LEU:HD23	0.52	2.28	16	1
1:A:183:PHE:CE2	1:A:199:LEU:HD11	0.52	2.40	20	1
1:A:266:TYR:CZ	1:A:267:LEU:HD12	0.52	2.40	3	2
1:A:199:LEU:O	1:A:199:LEU:HD13	0.52	2.05	7	1
1:A:149:LYS:HD2	1:A:158:LEU:HD12	0.52	1.82	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:LEU:HD13	1:A:266:TYR:CE1	0.51	2.40	2	1
1:A:158:LEU:HD22	1:A:158:LEU:N	0.51	2.20	18	3
1:A:215:ARG:NH2	1:A:227:LEU:HD23	0.51	2.20	5	1
1:A:195:PHE:CE1	1:A:199:LEU:HD12	0.51	2.40	2	1
1:A:170:LEU:HD21	1:A:200:ALA:CA	0.51	2.35	9	1
1:A:214:LEU:HD13	1:A:252:TYR:CZ	0.51	2.40	6	3
1:A:267:LEU:O	1:A:267:LEU:HD23	0.51	2.05	18	1
1:A:196:ALA:HB1	1:A:250:LEU:HD13	0.51	1.83	2	1
1:A:168:VAL:HG11	1:A:250:LEU:HD12	0.51	1.81	10	2
1:A:220:THR:HA	1:A:263:VAL:HG21	0.51	1.81	4	1
1:A:153:ASP:HB2	1:A:181:MET:HE3	0.51	1.82	8	1
1:A:189:ILE:HD13	1:A:226:PRO:O	0.50	2.06	10	6
1:A:149:LYS:HE3	1:A:158:LEU:HD22	0.50	1.84	5	1
1:A:148:LEU:HD11	1:A:167:GLN:OE1	0.50	2.07	8	1
1:A:164:ILE:HG21	1:A:185:HIS:CD2	0.50	2.41	12	1
1:A:170:LEU:O	1:A:267:LEU:HD21	0.50	2.05	19	1
1:A:197:ALA:HB1	1:A:202:LEU:O	0.50	2.06	9	1
1:A:170:LEU:HD13	1:A:179:LYS:HB2	0.50	1.82	6	1
1:A:214:LEU:HD12	1:A:252:TYR:N	0.49	2.23	1	2
1:A:183:PHE:CD1	1:A:199:LEU:HD13	0.49	2.43	3	1
1:A:251:GLU:HG2	1:A:253:LEU:HD12	0.49	1.85	12	1
1:A:185:HIS:NE2	1:A:231:LEU:HD11	0.49	2.23	2	1
1:A:231:LEU:C	1:A:235:ILE:HD12	0.49	2.33	7	1
1:A:171:PRO:HA	1:A:267:LEU:HD21	0.49	1.84	9	1
1:A:145:LEU:HD13	1:A:158:LEU:CD1	0.49	2.38	11	1
1:A:158:LEU:HD12	1:A:182:PHE:CE1	0.48	2.43	5	1
1:A:148:LEU:HD23	1:A:165:TYR:HB2	0.48	1.85	14	3
1:A:145:LEU:HD12	1:A:146:MET:N	0.48	2.23	11	1
1:A:181:MET:HG3	1:A:199:LEU:HD13	0.48	1.84	16	1
1:A:216:LEU:HD12	1:A:225:LEU:HD23	0.48	1.85	12	1
1:A:219:ILE:HG23	1:A:220:THR:HG23	0.48	1.86	18	1
1:A:193:ILE:HD13	1:A:213:LYS:NZ	0.48	2.23	13	1
1:A:145:LEU:HD21	1:A:158:LEU:HD22	0.48	1.86	2	1
1:A:193:ILE:HG23	1:A:215:ARG:HA	0.47	1.85	7	1
1:A:251:GLU:OE2	1:A:253:LEU:HD13	0.47	2.10	20	2
1:A:209:PHE:O	1:A:210:THR:HG22	0.47	2.09	16	1
1:A:183:PHE:CE1	1:A:199:LEU:HD13	0.47	2.44	3	1
1:A:169:PHE:O	1:A:267:LEU:HD11	0.47	2.10	4	1
1:A:214:LEU:HD12	1:A:251:GLU:C	0.47	2.35	1	4
1:A:168:VAL:HG12	1:A:170:LEU:HD22	0.47	1.86	12	3
1:A:170:LEU:HD13	1:A:179:LYS:CG	0.47	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:PHE:O	1:A:169:PHE:CG	0.47	2.66	17	1
1:A:250:LEU:O	1:A:267:LEU:HD11	0.47	2.10	15	1
1:A:216:LEU:O	1:A:216:LEU:HD22	0.47	2.10	14	4
1:A:170:LEU:HD13	1:A:179:LYS:CB	0.46	2.40	6	1
1:A:158:LEU:CD1	1:A:158:LEU:N	0.46	2.78	11	1
1:A:193:ILE:HD13	1:A:215:ARG:HD2	0.46	1.86	19	1
1:A:253:LEU:HD23	1:A:254:ASN:N	0.46	2.26	5	1
1:A:158:LEU:HD13	1:A:163:ARG:CD	0.46	2.41	14	1
1:A:145:LEU:HD21	1:A:158:LEU:HD11	0.46	1.86	10	1
1:A:197:ALA:HB2	1:A:204:ASN:OD1	0.46	2.11	9	1
1:A:261:LYS:C	1:A:262:ASN:CG	0.46	2.84	17	15
1:A:145:LEU:HD21	1:A:165:TYR:OH	0.46	2.11	4	1
1:A:181:MET:CE	1:A:199:LEU:HD13	0.46	2.25	15	1
1:A:181:MET:HB3	1:A:199:LEU:HD11	0.45	1.86	1	1
1:A:202:LEU:HD12	1:A:203:LYS:C	0.45	2.36	18	1
1:A:266:TYR:CD2	1:A:267:LEU:HD13	0.45	2.46	9	1
1:A:149:LYS:CE	1:A:158:LEU:HD22	0.45	2.42	5	1
1:A:196:ALA:HB1	1:A:250:LEU:CD1	0.45	2.42	2	1
1:A:196:ALA:HB2	1:A:250:LEU:CD1	0.45	2.42	14	1
1:A:168:VAL:HG21	1:A:181:MET:HE1	0.45	1.89	19	1
1:A:215:ARG:HH22	1:A:227:LEU:HD23	0.45	1.71	5	1
1:A:168:VAL:HG12	1:A:170:LEU:HD12	0.45	1.88	9	1
1:A:193:ILE:HD13	1:A:215:ARG:HG2	0.45	1.87	2	2
1:A:156:LYS:O	1:A:158:LEU:HD22	0.45	2.12	7	1
1:A:193:ILE:HD13	1:A:216:LEU:HD23	0.45	1.88	16	1
1:A:158:LEU:CD2	1:A:158:LEU:O	0.45	2.65	18	1
1:A:171:PRO:HA	1:A:267:LEU:HD11	0.45	1.88	3	1
1:A:143:VAL:HG13	1:A:146:MET:HE2	0.44	1.89	8	1
1:A:250:LEU:O	1:A:267:LEU:HD21	0.44	2.13	14	1
1:A:158:LEU:HD23	1:A:160:GLN:O	0.44	2.13	11	1
1:A:192:ALA:CB	1:A:216:LEU:HD21	0.44	2.42	11	1
1:A:196:ALA:HB1	1:A:250:LEU:HD21	0.44	1.88	1	1
1:A:170:LEU:HD12	1:A:179:LYS:HD2	0.44	1.89	11	1
1:A:189:ILE:HD12	1:A:229:HIS:O	0.44	2.12	16	2
1:A:186:ARG:NH1	1:A:235:ILE:HD13	0.44	2.27	20	1
1:A:183:PHE:CD1	1:A:183:PHE:N	0.44	2.85	14	1
1:A:224:ALA:HB2	1:A:258:GLN:O	0.44	2.13	16	1
1:A:193:ILE:HD13	1:A:215:ARG:CZ	0.44	2.43	8	1
1:A:171:PRO:HB3	1:A:267:LEU:HD11	0.44	1.88	16	2
1:A:214:LEU:HD21	1:A:250:LEU:HB3	0.44	1.90	17	1
1:A:168:VAL:CG1	1:A:250:LEU:HD23	0.44	2.40	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:261:LYS:O	1:A:262:ASN:C	0.44	2.60	6	16
1:A:216:LEU:HA	1:A:250:LEU:HD23	0.44	1.90	12	1
1:A:225:LEU:HD13	1:A:231:LEU:CD2	0.43	2.38	8	1
1:A:145:LEU:HD13	1:A:158:LEU:HD11	0.43	1.90	11	1
1:A:253:LEU:HD22	1:A:260:CYS:SG	0.43	2.52	9	3
1:A:234:TRP:O	1:A:237:LYS:HB2	0.43	2.13	13	1
1:A:187:TRP:C	1:A:230:THR:HG23	0.43	2.38	16	1
1:A:168:VAL:HG13	1:A:250:LEU:CD1	0.43	2.43	2	1
1:A:181:MET:SD	1:A:199:LEU:HD13	0.43	2.53	5	1
1:A:221:SER:H	1:A:263:VAL:HG11	0.43	1.73	12	1
1:A:158:LEU:N	1:A:158:LEU:HD13	0.43	2.28	11	1
1:A:145:LEU:HD11	1:A:165:TYR:HE1	0.43	1.72	14	1
1:A:145:LEU:CD2	1:A:158:LEU:HD21	0.43	2.44	20	1
1:A:181:MET:SD	1:A:199:LEU:HD22	0.43	2.54	5	1
1:A:170:LEU:HD21	1:A:179:LYS:HB2	0.43	1.90	1	2
1:A:214:LEU:CG	1:A:250:LEU:HD22	0.42	2.44	10	1
1:A:186:ARG:O	1:A:230:THR:HG22	0.42	2.14	20	1
1:A:158:LEU:HD13	1:A:163:ARG:HD2	0.42	1.91	16	1
1:A:158:LEU:HD13	1:A:163:ARG:NE	0.42	2.29	14	1
1:A:185:HIS:CD2	1:A:185:HIS:C	0.42	2.98	12	1
1:A:181:MET:HE3	1:A:199:LEU:HD21	0.42	1.91	3	1
1:A:168:VAL:HG12	1:A:170:LEU:CD2	0.42	2.45	4	1
1:A:170:LEU:HD21	1:A:179:LYS:CG	0.42	2.45	1	1
1:A:182:PHE:C	1:A:183:PHE:CG	0.42	2.98	14	1
1:A:170:LEU:HD12	1:A:179:LYS:HG3	0.42	1.91	15	1
1:A:240:CYS:SG	1:A:242:LEU:HD23	0.42	2.55	19	1
1:A:253:LEU:HD13	1:A:260:CYS:SG	0.41	2.55	4	1
1:A:145:LEU:HD23	1:A:146:MET:N	0.41	2.29	19	1
1:A:196:ALA:CB	1:A:250:LEU:HD11	0.41	2.46	20	1
1:A:149:LYS:NZ	1:A:158:LEU:HD22	0.41	2.30	5	1
1:A:158:LEU:C	1:A:158:LEU:CD2	0.41	2.86	11	2
1:A:160:GLN:N	1:A:160:GLN:CD	0.41	2.79	12	1
1:A:214:LEU:HG	1:A:250:LEU:HD12	0.41	1.91	20	1
1:A:164:ILE:HG23	1:A:185:HIS:CE1	0.41	2.50	3	1
1:A:202:LEU:HG	1:A:214:LEU:HD22	0.41	1.91	3	1
1:A:170:LEU:HD22	1:A:179:LYS:HD3	0.41	1.91	9	1
1:A:158:LEU:HD12	1:A:163:ARG:HB2	0.41	1.92	17	1
1:A:153:ASP:OD2	1:A:199:LEU:HD21	0.41	2.16	19	1
1:A:196:ALA:CB	1:A:250:LEU:HD21	0.41	2.46	1	1
1:A:267:LEU:O	1:A:268:GLU:C	0.41	2.63	9	1
1:A:170:LEU:HD22	1:A:179:LYS:CD	0.40	2.46	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:ALA:HB3	1:A:204:ASN:ND2	0.40	2.32	1	1
1:A:170:LEU:HD13	1:A:179:LYS:HD3	0.40	1.93	9	1
1:A:193:ILE:HA	1:A:216:LEU:HD11	0.40	1.91	1	1
1:A:216:LEU:HD23	1:A:225:LEU:HB2	0.40	1.94	1	1
1:A:166:PHE:CE1	1:A:168:VAL:HG22	0.40	2.51	8	2
1:A:202:LEU:C	1:A:202:LEU:HD12	0.40	2.42	10	1
1:A:234:TRP:CB	1:A:242:LEU:HD21	0.40	2.46	13	1
1:A:181:MET:SD	1:A:199:LEU:HD21	0.40	2.57	4	1
1:A:266:TYR:CD1	1:A:267:LEU:HD23	0.40	2.52	6	2

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/139 (96%)	113±3 (85±2%)	15±3 (11±2%)	5±2 (4±1%)	4	30
All	All	2660/2780 (96%)	2254 (85%)	303 (11%)	103 (4%)	4	30

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	262	ASN	18
1	A	152	ALA	16
1	A	210	THR	8
1	A	136	ASN	8
1	A	187	TRP	7
1	A	207	ASN	5
1	A	174	SER	5
1	A	257	GLU	4
1	A	221	SER	4
1	A	258	GLN	4
1	A	135	LYS	3
1	A	211	ALA	3
1	A	159	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	173	GLY	2
1	A	205	ASP	2
1	A	209	PHE	2
1	A	160	GLN	2
1	A	208	LYS	2
1	A	206	ASN	2
1	A	204	ASN	1
1	A	241	PRO	1
1	A	158	LEU	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/118 (99%)	80±3 (69±3%)	37±3 (31±3%)	1	14
All	All	2340/2360 (99%)	1605 (69%)	735 (31%)	1	14

All 94 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	216	LEU	20
1	A	261	LYS	20
1	A	150	MET	19
1	A	237	LYS	18
1	A	155	ASP	17
1	A	267	LEU	17
1	A	181	MET	16
1	A	212	LYS	16
1	A	221	SER	16
1	A	265	SER	16
1	A	163	ARG	15
1	A	191	LYS	15
1	A	262	ASN	15
1	A	156	LYS	15
1	A	213	LYS	15
1	A	227	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	136	ASN	14
1	A	165	TYR	14
1	A	230	THR	14
1	A	174	SER	14
1	A	187	TRP	14
1	A	214	LEU	13
1	A	158	LEU	12
1	A	160	GLN	12
1	A	199	LEU	12
1	A	135	LYS	11
1	A	177	LYS	11
1	A	218	HIS	11
1	A	183	PHE	10
1	A	198	SER	10
1	A	248	ILE	10
1	A	145	LEU	9
1	A	149	LYS	9
1	A	209	PHE	9
1	A	239	ASP	9
1	A	251	GLU	9
1	A	253	LEU	9
1	A	148	LEU	9
1	A	242	LEU	9
1	A	258	GLN	9
1	A	137	SER	8
1	A	178	SER	8
1	A	256	GLU	8
1	A	208	LYS	8
1	A	257	GLU	8
1	A	238	GLU	7
1	A	147	LYS	7
1	A	172	LYS	7
1	A	206	ASN	7
1	A	164	ILE	7
1	A	220	THR	7
1	A	207	ASN	6
1	A	250	LEU	6
1	A	202	LEU	6
1	A	205	ASP	5
1	A	167	GLN	5
1	A	228	ASP	5
1	A	142	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	203	LYS	5
1	A	219	ILE	5
1	A	179	LYS	5
1	A	138	GLU	4
1	A	185	HIS	4
1	A	162	GLU	4
1	A	195	PHE	4
1	A	210	THR	4
1	A	153	ASP	4
1	A	215	ARG	4
1	A	176	GLU	4
1	A	188	SER	3
1	A	186	ARG	3
1	A	243	TYR	3
1	A	194	ASP	3
1	A	259	PHE	2
1	A	223	GLU	2
1	A	249	ILE	2
1	A	240	CYS	2
1	A	175	LYS	2
1	A	232	GLU	2
1	A	266	TYR	2
1	A	244	ASN	1
1	A	255	ASP	1
1	A	201	ARG	1
1	A	217	CYS	1
1	A	247	ASN	1
1	A	268	GLU	1
1	A	204	ASN	1
1	A	182	PHE	1
1	A	169	PHE	1
1	A	254	ASN	1
1	A	157	SER	1
1	A	161	THR	1
1	A	260	CYS	1
1	A	235	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1558
Number of shifts mapped to atoms	1558
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	-0.05 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	-0.02 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.13 ± 0.14	None needed (< 0.5 ppm)
^{15}N	133	0.29 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1533 atoms were assigned a chemical shift out of a possible 1853. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	626/666 (94%)	263/269 (98%)	234/268 (87%)	129/129 (100%)
Sidechain	848/1029 (82%)	572/665 (86%)	266/325 (82%)	10/39 (26%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	59/158 (37%)	39/79 (49%)	20/73 (27%)	0/6 (0%)
Overall	1533/1853 (83%)	874/1013 (86%)	520/666 (78%)	139/174 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1558 atoms were assigned a chemical shift out of a possible 1888. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	644/694 (93%)	273/282 (97%)	238/278 (86%)	133/134 (99%)
Sidechain	855/1036 (83%)	577/670 (86%)	268/327 (82%)	10/39 (26%)
Aromatic	59/158 (37%)	39/79 (49%)	20/73 (27%)	0/6 (0%)
Overall	1558/1888 (83%)	889/1031 (86%)	526/678 (78%)	143/179 (80%)

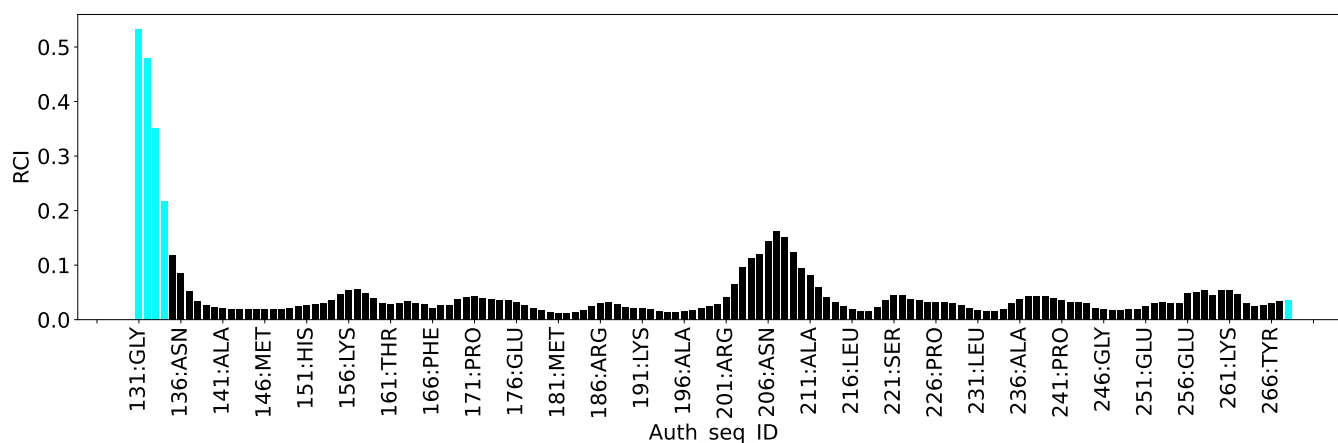
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1067
Intra-residue ($ i-j =0$)	263
Sequential ($ i-j =1$)	370
Medium range ($ i-j >1$ and $ i-j <5$)	182
Long range ($ i-j \geq 5$)	252
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.7
Number of long range restraints per residue ¹	1.8

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.5	0.2
0.2-0.5 (Medium)	1.6	0.5
>0.5 (Large)	0.1	0.57

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

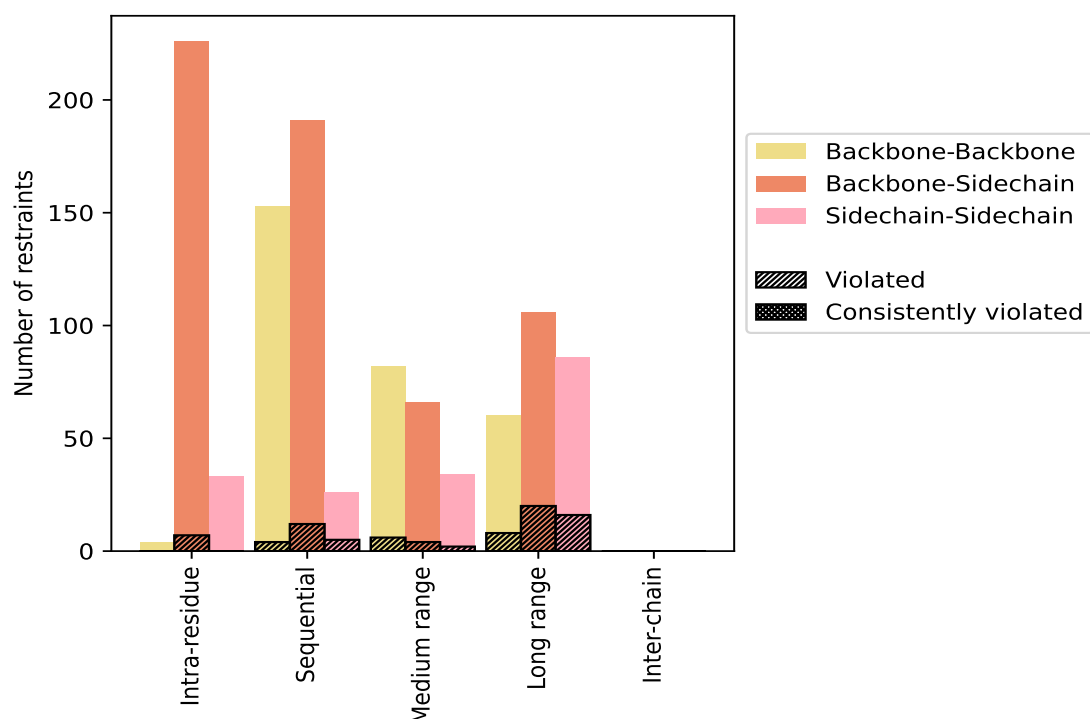
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	263	24.6	7	2.7	0.7	0	0.0	0.0
Backbone-Backbone	4	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	226	21.2	7	3.1	0.7	0	0.0	0.0
Sidechain-Sidechain	33	3.1	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	370	34.7	21	5.7	2.0	0	0.0	0.0
Backbone-Backbone	153	14.3	4	2.6	0.4	0	0.0	0.0
Backbone-Sidechain	191	17.9	12	6.3	1.1	0	0.0	0.0
Sidechain-Sidechain	26	2.4	5	19.2	0.5	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	182	17.1	12	6.6	1.1	0	0.0	0.0
Backbone-Backbone	82	7.7	6	7.3	0.6	0	0.0	0.0
Backbone-Sidechain	66	6.2	4	6.1	0.4	0	0.0	0.0
Sidechain-Sidechain	34	3.2	2	5.9	0.2	0	0.0	0.0
Long range (i-j ≥5)	252	23.6	44	17.5	4.1	0	0.0	0.0
Backbone-Backbone	60	5.6	8	13.3	0.7	0	0.0	0.0
Backbone-Sidechain	106	9.9	20	18.9	1.9	0	0.0	0.0
Sidechain-Sidechain	86	8.1	16	18.6	1.5	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1067	100.0	84	7.9	7.9	0	0.0	0.0
Backbone-Backbone	299	28.0	18	6.0	1.7	0	0.0	0.0
Backbone-Sidechain	589	55.2	43	7.3	4.0	0	0.0	0.0
Sidechain-Sidechain	179	16.8	23	12.8	2.2	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	3	1	11	0	16	0.17	0.3	0.06	0.15
2	0	1	2	0	0	3	0.12	0.13	0.01	0.11
3	1	2	0	0	0	3	0.2	0.31	0.08	0.18
4	0	1	2	3	0	6	0.14	0.19	0.03	0.13
5	0	0	1	2	0	3	0.12	0.14	0.01	0.12
6	0	1	1	3	0	5	0.12	0.13	0.01	0.12
7	0	0	0	4	0	4	0.13	0.16	0.03	0.13
8	0	0	0	4	0	4	0.15	0.18	0.02	0.15
9	0	4	3	3	0	10	0.16	0.25	0.05	0.16
10	1	2	1	6	0	10	0.14	0.24	0.05	0.12

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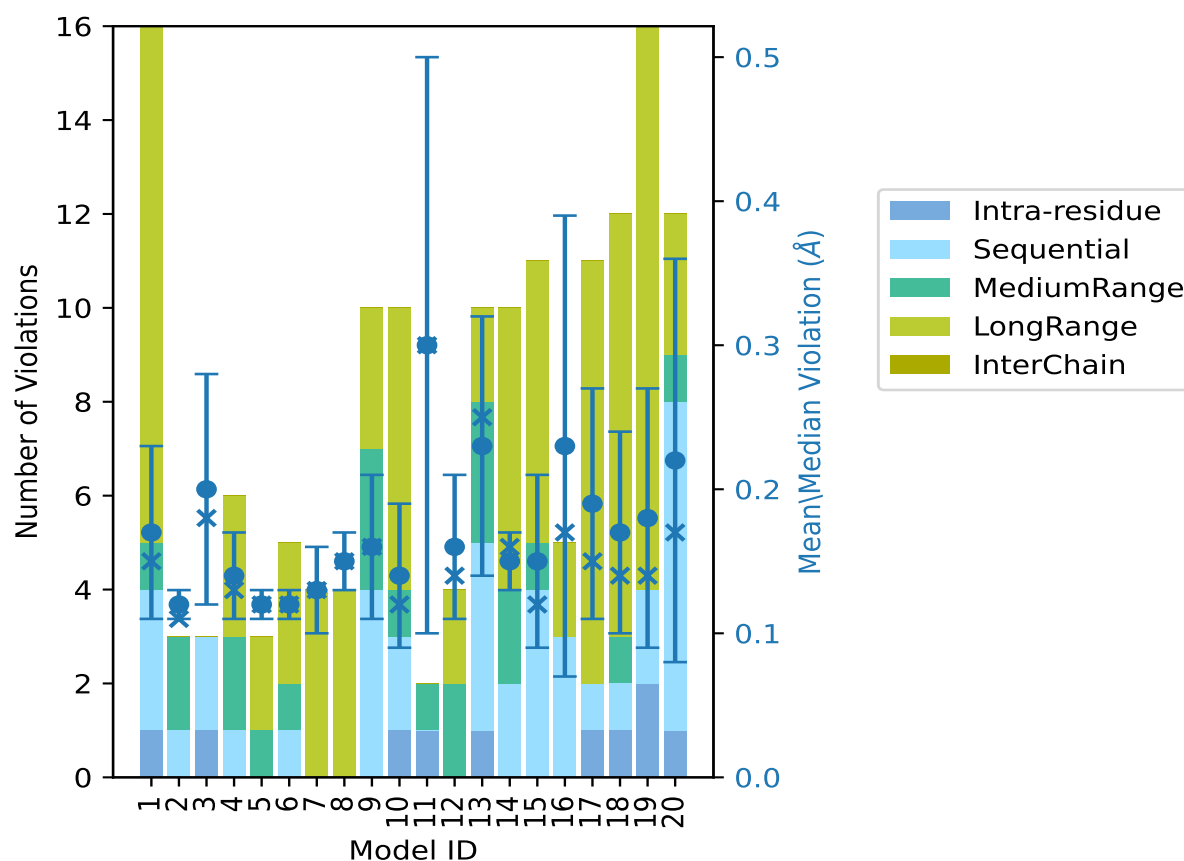
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	0	1	0	0	2	0.3	0.5	0.2	0.3
12	0	0	2	2	0	4	0.16	0.24	0.05	0.14
13	1	4	3	2	0	10	0.23	0.37	0.09	0.25
14	0	2	2	6	0	10	0.15	0.2	0.02	0.16
15	0	4	1	6	0	11	0.15	0.31	0.06	0.12
16	0	3	0	2	0	5	0.23	0.55	0.16	0.17
17	1	1	0	9	0	11	0.19	0.4	0.08	0.15
18	1	1	1	9	0	12	0.17	0.31	0.07	0.14
19	2	2	0	12	0	16	0.18	0.39	0.09	0.14
20	1	7	1	3	0	12	0.22	0.57	0.14	0.17

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

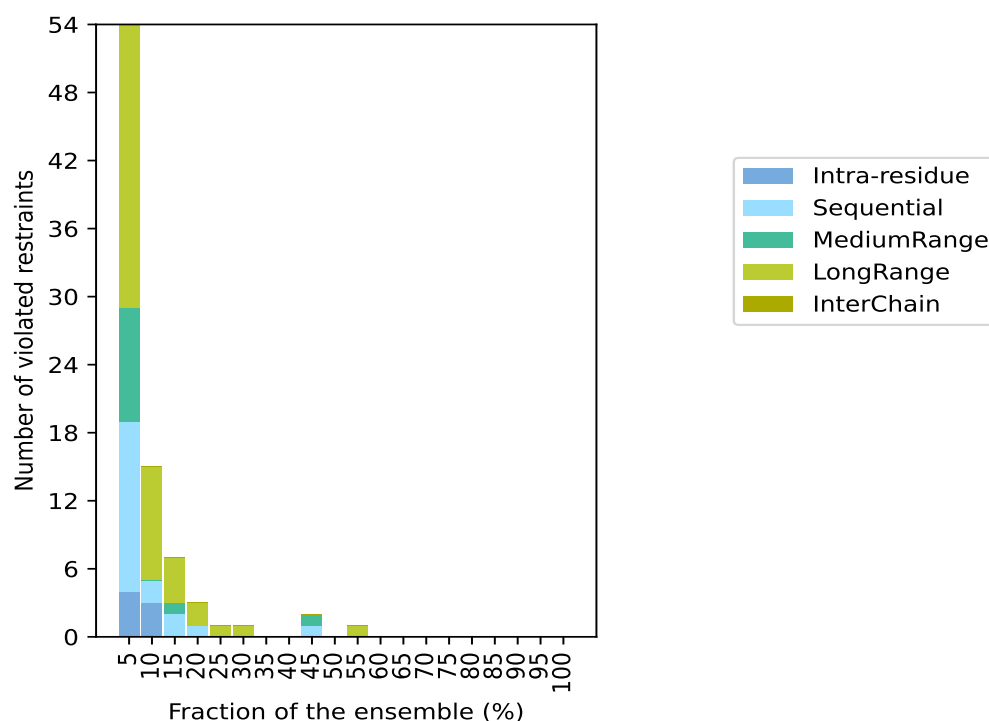
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 983(IR:256, SQ:349, MR:170, LR:208, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	15	10	25	0	54	1	5.0
3	2	0	10	0	15	2	10.0
0	2	1	4	0	7	3	15.0
0	1	0	2	0	3	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	1	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	1	1	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

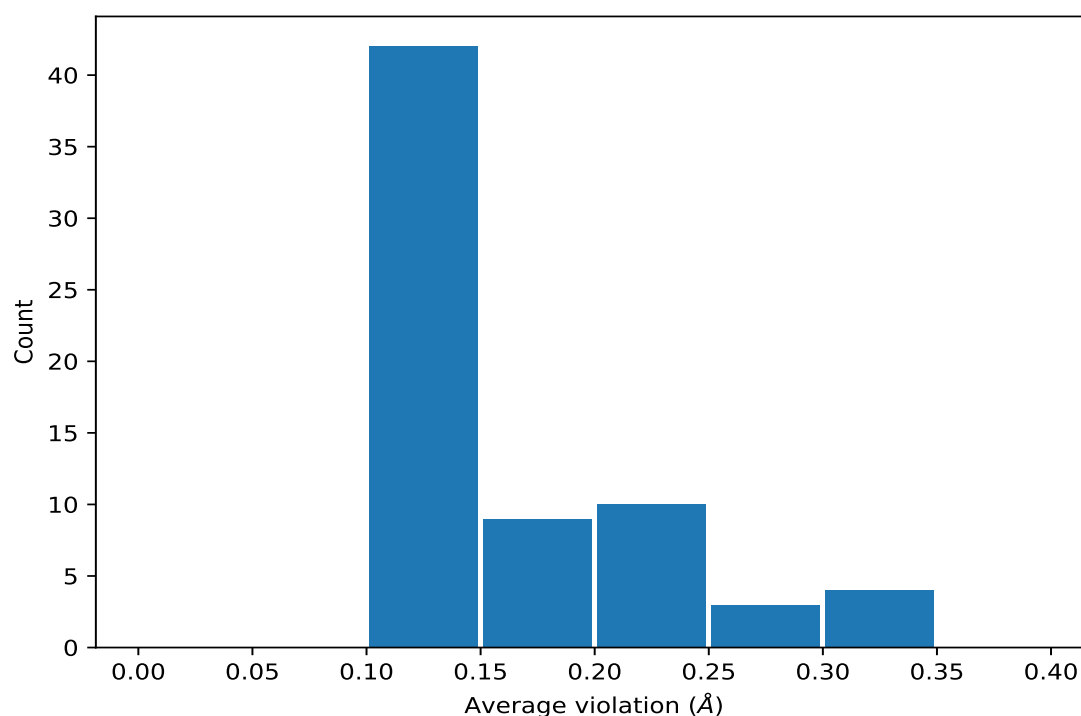
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	11	0.16	0.05	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	11	0.16	0.05	0.15
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	9	0.18	0.01	0.18
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	9	0.11	0.01	0.11
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	9	0.11	0.01	0.11
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	9	0.11	0.01	0.11
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	6	0.19	0.05	0.19
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	5	0.16	0.05	0.13
(1,798)	1:166:A:PHE:H	1:181:A:MET:H	4	0.29	0.04	0.29
(1,596)	1:157:A:SER:H	1:158:A:LEU:H	4	0.24	0.05	0.24
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB2	4	0.12	0.02	0.12
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB3	4	0.12	0.02	0.12
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB2	4	0.12	0.02	0.12
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB3	4	0.12	0.02	0.12
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE1	3	0.21	0.13	0.12
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE2	3	0.21	0.13	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE3	3	0.21	0.13	0.12
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG2	3	0.13	0.02	0.14
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG3	3	0.13	0.02	0.14
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG2	3	0.13	0.02	0.14
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG3	3	0.13	0.02	0.14
(1,942)	1:209:A:PHE:HB2	1:210:A:THR:H	3	0.12	0.0	0.12
(1,942)	1:209:A:PHE:HB3	1:210:A:THR:H	3	0.12	0.0	0.12
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD1	3	0.12	0.01	0.12
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD2	3	0.12	0.01	0.12
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD1	3	0.12	0.01	0.12
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD2	3	0.12	0.01	0.12
(1,629)	1:236:A:ALA:H	1:237:A:LYS:HA	3	0.12	0.02	0.11
(1,809)	1:224:A:ALA:H	1:259:A:PHE:H	3	0.11	0.0	0.11
(1,311)	1:135:A:LYS:HA	1:138:A:GLU:H	3	0.11	0.0	0.11
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG2	2	0.32	0.18	0.32
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG3	2	0.32	0.18	0.32
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG2	2	0.31	0.0	0.31
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG3	2	0.31	0.0	0.31
(1,447)	1:169:A:PHE:HD1	1:248:A:ILE:HA	2	0.27	0.13	0.27
(1,447)	1:169:A:PHE:HD2	1:248:A:ILE:HA	2	0.27	0.13	0.27
(1,191)	1:238:A:GLU:HB2	1:239:A:ASP:H	2	0.23	0.03	0.23
(1,191)	1:238:A:GLU:HB3	1:239:A:ASP:H	2	0.23	0.03	0.23
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB2	2	0.22	0.05	0.22
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB3	2	0.22	0.05	0.22
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB2	2	0.22	0.05	0.22
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB3	2	0.22	0.05	0.22
(1,1009)	1:149:A:LYS:HB2	1:165:A:TYR:HE2	2	0.18	0.02	0.18
(1,1009)	1:149:A:LYS:HB3	1:165:A:TYR:HE2	2	0.18	0.02	0.18
(1,496)	1:189:A:ILE:HG12	1:225:A:LEU:HG	2	0.16	0.02	0.16
(1,496)	1:189:A:ILE:HG13	1:225:A:LEU:HG	2	0.16	0.02	0.16
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB2	2	0.15	0.01	0.15
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB3	2	0.15	0.01	0.15
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB2	2	0.15	0.01	0.15
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB3	2	0.15	0.01	0.15
(1,362)	1:164:A:ILE:H	1:185:A:HIS:H	2	0.15	0.02	0.15
(1,243)	1:148:A:LEU:HD11	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,243)	1:148:A:LEU:HD12	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,243)	1:148:A:LEU:HD13	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,243)	1:148:A:LEU:HD21	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,243)	1:148:A:LEU:HD22	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,243)	1:148:A:LEU:HD23	1:167:A:GLN:H	2	0.14	0.04	0.14
(1,805)	1:152:A:ALA:HB1	1:182:A:PHE:H	2	0.14	0.02	0.14

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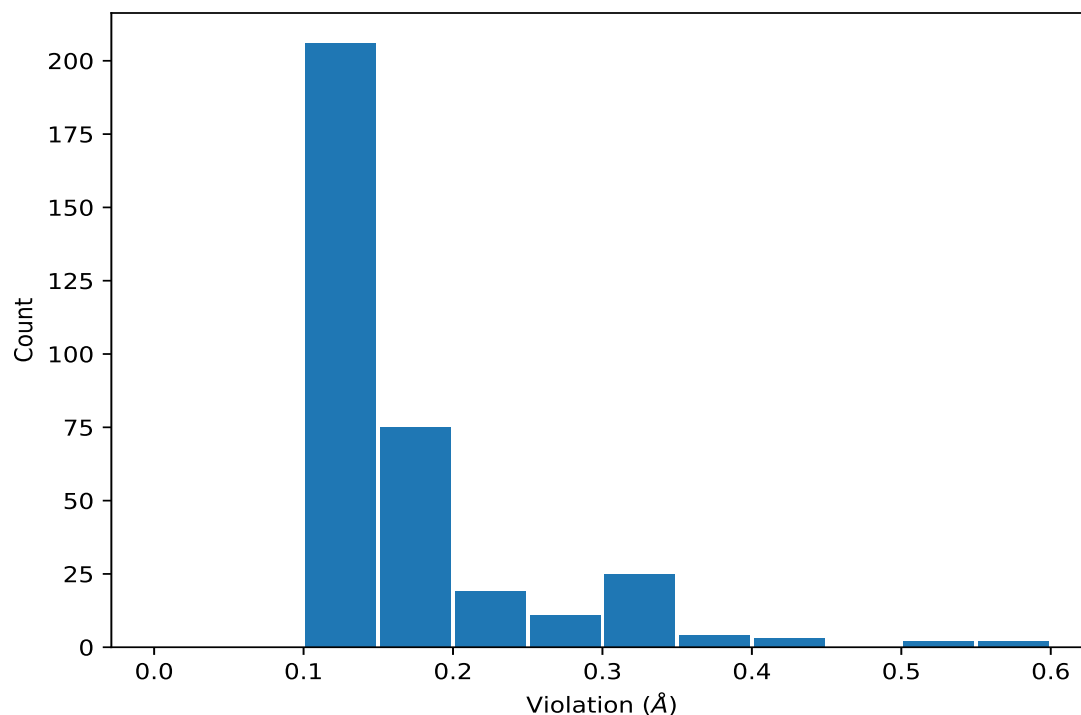
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,805)	1:152:A:ALA:HB2	1:182:A:PHE:H	2	0.14	0.02	0.14
(1,805)	1:152:A:ALA:HB3	1:182:A:PHE:H	2	0.14	0.02	0.14
(1,828)	1:148:A:LEU:HG	1:166:A:PHE:H	2	0.12	0.01	0.12
(1,1020)	1:265:A:SER:H	1:266:A:TYR:HB3	2	0.12	0.0	0.12
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD1	2	0.11	0.0	0.11
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD2	2	0.11	0.0	0.11
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB2	2	0.11	0.0	0.11
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB3	2	0.11	0.0	0.11
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB2	2	0.11	0.0	0.11
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:237:A:LYS:H	1:237:A:LYS:HB2	20	0.57
(1,98)	1:185:A:HIS:H	1:186:A:ARG:HB2	16	0.55
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG2	11	0.5
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG3	11	0.5
(1,210)	1:237:A:LYS:HB3	1:239:A:ASP:H	20	0.41
(1,447)	1:169:A:PHE:HD1	1:248:A:ILE:HA	17	0.4
(1,447)	1:169:A:PHE:HD2	1:248:A:ILE:HA	17	0.4
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE1	19	0.39
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE2	19	0.39
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE3	19	0.39
(1,579)	1:237:A:LYS:H	1:242:A:LEU:HG	13	0.37
(1,798)	1:166:A:PHE:H	1:181:A:MET:H	19	0.34
(1,648)	1:176:A:GLU:HG2	1:177:A:LYS:HB2	20	0.34
(1,648)	1:176:A:GLU:HG2	1:177:A:LYS:HB3	20	0.34
(1,648)	1:176:A:GLU:HG3	1:177:A:LYS:HB2	20	0.34
(1,648)	1:176:A:GLU:HG3	1:177:A:LYS:HB3	20	0.34
(1,217)	1:239:A:ASP:HB2	1:240:A:CYS:HB2	13	0.32
(1,217)	1:239:A:ASP:HB2	1:240:A:CYS:HB3	13	0.32
(1,217)	1:239:A:ASP:HB3	1:240:A:CYS:HB2	13	0.32
(1,217)	1:239:A:ASP:HB3	1:240:A:CYS:HB3	13	0.32
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG2	3	0.31
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG3	3	0.31
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG2	13	0.31
(1,698)	1:177:A:LYS:H	1:177:A:LYS:HG3	13	0.31
(1,386)	1:163:A:ARG:HG2	1:164:A:ILE:HG21	15	0.31
(1,386)	1:163:A:ARG:HG2	1:164:A:ILE:HG22	15	0.31
(1,386)	1:163:A:ARG:HG2	1:164:A:ILE:HG23	15	0.31
(1,386)	1:163:A:ARG:HG3	1:164:A:ILE:HG21	15	0.31
(1,386)	1:163:A:ARG:HG3	1:164:A:ILE:HG22	15	0.31
(1,386)	1:163:A:ARG:HG3	1:164:A:ILE:HG23	15	0.31
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	19	0.31
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	19	0.31
(1,107)	1:158:A:LEU:H	1:163:A:ARG:HD2	18	0.31
(1,107)	1:158:A:LEU:H	1:163:A:ARG:HD3	18	0.31
(1,798)	1:166:A:PHE:H	1:181:A:MET:H	18	0.3
(1,596)	1:157:A:SER:H	1:158:A:LEU:H	1	0.3
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB2	17	0.27
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB3	17	0.27
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB2	17	0.27
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB3	17	0.27
(1,798)	1:166:A:PHE:H	1:181:A:MET:H	1	0.27
(1,191)	1:238:A:GLU:HB2	1:239:A:ASP:H	13	0.26
(1,191)	1:238:A:GLU:HB3	1:239:A:ASP:H	13	0.26
(1,875)	1:237:A:LYS:H	1:241:A:PRO:HA	13	0.25
(1,757)	1:234:A:TRP:HB3	1:237:A:LYS:HB3	13	0.25
(1,596)	1:157:A:SER:H	1:158:A:LEU:H	9	0.25
(1,798)	1:166:A:PHE:H	1:181:A:MET:H	10	0.24
(1,596)	1:157:A:SER:H	1:158:A:LEU:H	20	0.24
(1,361)	1:164:A:ILE:HD11	1:185:A:HIS:H	1	0.24
(1,361)	1:164:A:ILE:HD12	1:185:A:HIS:H	1	0.24
(1,361)	1:164:A:ILE:HD13	1:185:A:HIS:H	1	0.24
(1,265)	1:160:A:GLN:HE21	1:162:A:GLU:H	12	0.24
(1,265)	1:160:A:GLN:HE22	1:162:A:GLU:H	12	0.24
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	1	0.23
(1,69)	1:210:A:THR:HA	1:211:A:ALA:H	9	0.22
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	18	0.21
(1,382)	1:163:A:ARG:HG2	1:164:A:ILE:H	15	0.21
(1,382)	1:163:A:ARG:HG3	1:164:A:ILE:H	15	0.21
(1,235)	1:167:A:GLN:H	1:167:A:GLN:HE21	17	0.21
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	19	0.21
(1,1009)	1:149:A:LYS:HB2	1:165:A:TYR:HE2	19	0.2
(1,1009)	1:149:A:LYS:HB3	1:165:A:TYR:HE2	19	0.2
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	14	0.2
(1,191)	1:238:A:GLU:HB2	1:239:A:ASP:H	20	0.2
(1,191)	1:238:A:GLU:HB3	1:239:A:ASP:H	20	0.2
(1,937)	1:135:A:LYS:HA	1:139:A:THR:HA	4	0.19
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	1	0.19
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	10	0.19
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	1	0.19
(1,496)	1:189:A:ILE:HG12	1:225:A:LEU:HG	8	0.18
(1,496)	1:189:A:ILE:HG13	1:225:A:LEU:HG	8	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	3	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	4	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	9	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	14	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	16	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	17	0.18
(1,140)	1:205:A:ASP:HA	1:206:A:ASN:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB2	9	0.17
(1,831)	1:149:A:LYS:HD2	1:182:A:PHE:HB3	9	0.17
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB2	9	0.17
(1,831)	1:149:A:LYS:HD3	1:182:A:PHE:HB3	9	0.17
(1,822)	1:164:A:ILE:H	1:182:A:PHE:HB2	14	0.17
(1,822)	1:164:A:ILE:H	1:182:A:PHE:HB3	14	0.17
(1,606)	1:187:A:TRP:H	1:231:A:LEU:HB2	16	0.17
(1,606)	1:187:A:TRP:H	1:231:A:LEU:HB3	16	0.17
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	10	0.17
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	10	0.17
(1,243)	1:148:A:LEU:HD11	1:167:A:GLN:H	10	0.17
(1,243)	1:148:A:LEU:HD12	1:167:A:GLN:H	10	0.17
(1,243)	1:148:A:LEU:HD13	1:167:A:GLN:H	10	0.17
(1,243)	1:148:A:LEU:HD21	1:167:A:GLN:H	10	0.17
(1,243)	1:148:A:LEU:HD22	1:167:A:GLN:H	10	0.17
(1,243)	1:148:A:LEU:HD23	1:167:A:GLN:H	10	0.17
(1,1009)	1:149:A:LYS:HB2	1:165:A:TYR:HE2	1	0.16
(1,1009)	1:149:A:LYS:HB3	1:165:A:TYR:HE2	1	0.16
(1,830)	1:149:A:LYS:HE2	1:182:A:PHE:HB2	8	0.16
(1,830)	1:149:A:LYS:HE2	1:182:A:PHE:HB3	8	0.16
(1,830)	1:149:A:LYS:HE3	1:182:A:PHE:HB2	8	0.16
(1,830)	1:149:A:LYS:HE3	1:182:A:PHE:HB3	8	0.16
(1,805)	1:152:A:ALA:HB1	1:182:A:PHE:H	9	0.16
(1,805)	1:152:A:ALA:HB2	1:182:A:PHE:H	9	0.16
(1,805)	1:152:A:ALA:HB3	1:182:A:PHE:H	9	0.16
(1,680)	1:147:A:LYS:H	1:149:A:LYS:H	9	0.16
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB2	7	0.16
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB3	7	0.16
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB2	7	0.16
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB3	7	0.16
(1,362)	1:164:A:ILE:H	1:185:A:HIS:H	14	0.16
(1,339)	1:164:A:ILE:HA	1:245:A:GLY:H	17	0.16
(1,315)	1:237:A:LYS:HB3	1:238:A:GLU:H	20	0.16
(1,39)	1:193:A:ILE:HA	1:197:A:ALA:H	14	0.16
(1,998)	1:235:A:ILE:HG12	1:243:A:TYR:HD1	13	0.15
(1,998)	1:235:A:ILE:HG12	1:243:A:TYR:HD2	13	0.15
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	17	0.15
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB2	15	0.15
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB3	15	0.15
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB2	15	0.15
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB3	15	0.15
(1,689)	1:156:A:LYS:H	1:156:A:LYS:HD2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:156:A:LYS:H	1:156:A:LYS:HD3	18	0.15
(1,616)	1:168:A:VAL:HG11	1:250:A:LEU:HB3	17	0.15
(1,616)	1:168:A:VAL:HG12	1:250:A:LEU:HB3	17	0.15
(1,616)	1:168:A:VAL:HG13	1:250:A:LEU:HB3	17	0.15
(1,596)	1:157:A:SER:H	1:158:A:LEU:H	14	0.15
(1,397)	1:167:A:GLN:H	1:248:A:ILE:H	17	0.15
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	7	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	7	0.15
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	12	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	12	0.15
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	15	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	15	0.15
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	17	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	17	0.15
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	18	0.15
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	18	0.15
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG2	1	0.15
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG3	1	0.15
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG2	1	0.15
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG3	1	0.15
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD1	18	0.14
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD2	18	0.14
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD1	18	0.14
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD2	18	0.14
(1,992)	1:164:A:ILE:HG21	1:165:A:TYR:H	15	0.14
(1,992)	1:164:A:ILE:HG22	1:165:A:TYR:H	15	0.14
(1,992)	1:164:A:ILE:HG23	1:165:A:TYR:H	15	0.14
(1,923)	1:232:A:GLU:HG2	1:233:A:THR:H	19	0.14
(1,923)	1:232:A:GLU:HG3	1:233:A:THR:H	19	0.14
(1,854)	1:195:A:PHE:H	1:195:A:PHE:HD1	1	0.14
(1,854)	1:195:A:PHE:H	1:195:A:PHE:HD2	1	0.14
(1,755)	1:234:A:TRP:H	1:237:A:LYS:H	13	0.14
(1,736)	1:150:A:MET:HG2	1:156:A:LYS:HB2	18	0.14
(1,736)	1:150:A:MET:HG2	1:156:A:LYS:HB3	18	0.14
(1,736)	1:150:A:MET:HG3	1:156:A:LYS:HB2	18	0.14
(1,736)	1:150:A:MET:HG3	1:156:A:LYS:HB3	18	0.14
(1,629)	1:236:A:ALA:H	1:237:A:LYS:HA	16	0.14
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB2	19	0.14
(1,567)	1:149:A:LYS:HE2	1:158:A:LEU:HB3	19	0.14
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB2	19	0.14
(1,567)	1:149:A:LYS:HE3	1:158:A:LEU:HB3	19	0.14
(1,496)	1:189:A:ILE:HG12	1:225:A:LEU:HG	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:189:A:ILE:HG13	1:225:A:LEU:HG	14	0.14
(1,447)	1:169:A:PHE:HD1	1:248:A:ILE:HA	19	0.14
(1,447)	1:169:A:PHE:HD2	1:248:A:ILE:HA	19	0.14
(1,396)	1:167:A:GLN:HG2	1:248:A:ILE:H	4	0.14
(1,396)	1:167:A:GLN:HG3	1:248:A:ILE:H	4	0.14
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	5	0.14
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	5	0.14
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG2	8	0.14
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG3	8	0.14
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG2	8	0.14
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG3	8	0.14
(1,942)	1:209:A:PHE:HB2	1:210:A:THR:H	2	0.13
(1,942)	1:209:A:PHE:HB3	1:210:A:THR:H	2	0.13
(1,865)	1:165:A:TYR:H	1:183:A:PHE:H	6	0.13
(1,828)	1:148:A:LEU:HG	1:166:A:PHE:H	18	0.13
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB2	16	0.13
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB3	16	0.13
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB2	16	0.13
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB3	16	0.13
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	18	0.13
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	18	0.13
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	18	0.13
(1,632)	1:236:A:ALA:HB1	1:237:A:LYS:HG2	20	0.13
(1,632)	1:236:A:ALA:HB1	1:237:A:LYS:HG3	20	0.13
(1,632)	1:236:A:ALA:HB2	1:237:A:LYS:HG2	20	0.13
(1,632)	1:236:A:ALA:HB2	1:237:A:LYS:HG3	20	0.13
(1,632)	1:236:A:ALA:HB3	1:237:A:LYS:HG2	20	0.13
(1,632)	1:236:A:ALA:HB3	1:237:A:LYS:HG3	20	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD11	14	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD12	14	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD13	14	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD21	14	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD22	14	0.13
(1,587)	1:182:A:PHE:H	1:199:A:LEU:HD23	14	0.13
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	8	0.13
(1,391)	1:217:A:CYS:H	1:249:A:ILE:HB	18	0.13
(1,362)	1:164:A:ILE:H	1:185:A:HIS:H	12	0.13
(1,262)	1:217:A:CYS:H	1:251:A:GLU:H	14	0.13
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG2	19	0.13
(1,234)	1:167:A:GLN:H	1:167:A:GLN:HG3	19	0.13
(1,145)	1:164:A:ILE:HD11	1:244:A:ASN:HD21	1	0.13
(1,145)	1:164:A:ILE:HD11	1:244:A:ASN:HD22	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:164:A:ILE:HD12	1:244:A:ASN:HD21	1	0.13
(1,145)	1:164:A:ILE:HD12	1:244:A:ASN:HD22	1	0.13
(1,145)	1:164:A:ILE:HD13	1:244:A:ASN:HD21	1	0.13
(1,145)	1:164:A:ILE:HD13	1:244:A:ASN:HD22	1	0.13
(1,1020)	1:265:A:SER:H	1:266:A:TYR:HB3	6	0.12
(1,1020)	1:265:A:SER:H	1:266:A:TYR:HB3	20	0.12
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD1	6	0.12
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD2	6	0.12
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD1	6	0.12
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD2	6	0.12
(1,1001)	1:249:A:ILE:HD11	1:266:A:TYR:HE2	17	0.12
(1,1001)	1:249:A:ILE:HD12	1:266:A:TYR:HE2	17	0.12
(1,1001)	1:249:A:ILE:HD13	1:266:A:TYR:HE2	17	0.12
(1,942)	1:209:A:PHE:HB2	1:210:A:THR:H	10	0.12
(1,942)	1:209:A:PHE:HB3	1:210:A:THR:H	10	0.12
(1,942)	1:209:A:PHE:HB2	1:210:A:THR:H	13	0.12
(1,942)	1:209:A:PHE:HB3	1:210:A:THR:H	13	0.12
(1,899)	1:177:A:LYS:HD2	1:178:A:SER:H	18	0.12
(1,899)	1:177:A:LYS:HD3	1:178:A:SER:H	18	0.12
(1,809)	1:224:A:ALA:H	1:259:A:PHE:H	15	0.12
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE1	5	0.12
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE2	5	0.12
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE3	5	0.12
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	6	0.12
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	6	0.12
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	6	0.12
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	12	0.12
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	12	0.12
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	12	0.12
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	14	0.12
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	14	0.12
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	14	0.12
(1,510)	1:193:A:ILE:HA	1:216:A:LEU:HB2	1	0.12
(1,510)	1:193:A:ILE:HA	1:216:A:LEU:HB3	1	0.12
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	1	0.12
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	1	0.12
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	4	0.12
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	4	0.12
(1,51)	1:149:A:LYS:H	1:152:A:ALA:HB1	15	0.12
(1,51)	1:149:A:LYS:H	1:152:A:ALA:HB2	15	0.12
(1,51)	1:149:A:LYS:H	1:152:A:ALA:HB3	15	0.12
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD1	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:149:A:LYS:HB2	1:165:A:TYR:HD2	1	0.11
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD1	1	0.11
(1,1008)	1:149:A:LYS:HB3	1:165:A:TYR:HD2	1	0.11
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB2	10	0.11
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB3	10	0.11
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB2	10	0.11
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB3	10	0.11
(1,931)	1:219:A:ILE:HG12	1:220:A:THR:H	3	0.11
(1,931)	1:219:A:ILE:HG13	1:220:A:THR:H	3	0.11
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD1	19	0.11
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD2	19	0.11
(1,828)	1:148:A:LEU:HG	1:166:A:PHE:H	19	0.11
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB2	4	0.11
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB3	4	0.11
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB2	4	0.11
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB3	4	0.11
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB2	7	0.11
(1,820)	1:154:A:GLY:HA2	1:182:A:PHE:HB3	7	0.11
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB2	7	0.11
(1,820)	1:154:A:GLY:HA3	1:182:A:PHE:HB3	7	0.11
(1,809)	1:224:A:ALA:H	1:259:A:PHE:H	18	0.11
(1,809)	1:224:A:ALA:H	1:259:A:PHE:H	20	0.11
(1,805)	1:152:A:ALA:HB1	1:182:A:PHE:H	15	0.11
(1,805)	1:152:A:ALA:HB2	1:182:A:PHE:H	15	0.11
(1,805)	1:152:A:ALA:HB3	1:182:A:PHE:H	15	0.11
(1,783)	1:149:A:LYS:HB2	1:150:A:MET:HG2	9	0.11
(1,783)	1:149:A:LYS:HB2	1:150:A:MET:HG3	9	0.11
(1,783)	1:149:A:LYS:HB3	1:150:A:MET:HG2	9	0.11
(1,783)	1:149:A:LYS:HB3	1:150:A:MET:HG3	9	0.11
(1,771)	1:167:A:GLN:HA	1:181:A:MET:H	9	0.11
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE1	10	0.11
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE2	10	0.11
(1,766)	1:153:A:ASP:H	1:181:A:MET:HE3	10	0.11
(1,655)	1:145:A:LEU:HG	1:149:A:LYS:HB2	11	0.11
(1,655)	1:145:A:LEU:HG	1:149:A:LYS:HB3	11	0.11
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	1	0.11
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	1	0.11
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	1	0.11
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	2	0.11
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	2	0.11
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	2	0.11
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	5	0.11
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	5	0.11
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	9	0.11
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	9	0.11
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	9	0.11
(1,629)	1:236:A:ALA:H	1:237:A:LYS:HA	13	0.11
(1,540)	1:214:A:LEU:HD11	1:267:A:LEU:HG	19	0.11
(1,540)	1:214:A:LEU:HD12	1:267:A:LEU:HG	19	0.11
(1,540)	1:214:A:LEU:HD13	1:267:A:LEU:HG	19	0.11
(1,540)	1:214:A:LEU:HD21	1:267:A:LEU:HG	19	0.11
(1,540)	1:214:A:LEU:HD22	1:267:A:LEU:HG	19	0.11
(1,540)	1:214:A:LEU:HD23	1:267:A:LEU:HG	19	0.11
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	15	0.11
(1,507)	1:193:A:ILE:HB	1:216:A:LEU:H	20	0.11
(1,438)	1:166:A:PHE:HD1	1:248:A:ILE:HD11	19	0.11
(1,438)	1:166:A:PHE:HD1	1:248:A:ILE:HD12	19	0.11
(1,438)	1:166:A:PHE:HD1	1:248:A:ILE:HD13	19	0.11
(1,438)	1:166:A:PHE:HD2	1:248:A:ILE:HD11	19	0.11
(1,438)	1:166:A:PHE:HD2	1:248:A:ILE:HD12	19	0.11
(1,438)	1:166:A:PHE:HD2	1:248:A:ILE:HD13	19	0.11
(1,311)	1:135:A:LYS:HA	1:138:A:GLU:H	2	0.11
(1,311)	1:135:A:LYS:HA	1:138:A:GLU:H	9	0.11
(1,247)	1:166:A:PHE:HD1	1:167:A:GLN:H	1	0.11
(1,247)	1:166:A:PHE:HD2	1:167:A:GLN:H	1	0.11
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG2	19	0.11
(1,104)	1:164:A:ILE:HG12	1:186:A:ARG:HG3	19	0.11
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG2	19	0.11
(1,104)	1:164:A:ILE:HG13	1:186:A:ARG:HG3	19	0.11
(1,1019)	1:171:A:PRO:HB2	1:252:A:TYR:HD1	17	0.1
(1,1019)	1:171:A:PRO:HB2	1:252:A:TYR:HD2	17	0.1
(1,1019)	1:171:A:PRO:HB3	1:252:A:TYR:HD1	17	0.1
(1,1019)	1:171:A:PRO:HB3	1:252:A:TYR:HD2	17	0.1
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB2	19	0.1
(1,1003)	1:148:A:LEU:HB2	1:165:A:TYR:HB3	19	0.1
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB2	19	0.1
(1,1003)	1:148:A:LEU:HB3	1:165:A:TYR:HB3	19	0.1
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD1	10	0.1
(1,842)	1:166:A:PHE:HA	1:166:A:PHE:HD2	10	0.1
(1,838)	1:166:A:PHE:H	1:182:A:PHE:HB2	15	0.1
(1,838)	1:166:A:PHE:H	1:182:A:PHE:HB3	15	0.1
(1,650)	1:235:A:ILE:HG21	1:237:A:LYS:H	10	0.1
(1,650)	1:235:A:ILE:HG22	1:237:A:LYS:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:235:A:ILE:HG23	1:237:A:LYS:H	10	0.1
(1,629)	1:236:A:ALA:H	1:237:A:LYS:HA	10	0.1
(1,569)	1:149:A:LYS:HD2	1:158:A:LEU:H	7	0.1
(1,569)	1:149:A:LYS:HD3	1:158:A:LEU:H	7	0.1
(1,506)	1:193:A:ILE:H	1:216:A:LEU:HG	6	0.1
(1,342)	1:166:A:PHE:HD1	1:246:A:GLY:H	20	0.1
(1,342)	1:166:A:PHE:HD2	1:246:A:GLY:H	20	0.1
(1,311)	1:135:A:LYS:HA	1:138:A:GLU:H	4	0.1
(1,243)	1:148:A:LEU:HD11	1:167:A:GLN:H	1	0.1
(1,243)	1:148:A:LEU:HD12	1:167:A:GLN:H	1	0.1
(1,243)	1:148:A:LEU:HD13	1:167:A:GLN:H	1	0.1
(1,243)	1:148:A:LEU:HD21	1:167:A:GLN:H	1	0.1
(1,243)	1:148:A:LEU:HD22	1:167:A:GLN:H	1	0.1
(1,243)	1:148:A:LEU:HD23	1:167:A:GLN:H	1	0.1
(1,96)	1:162:A:GLU:H	1:163:A:ARG:HB2	15	0.1
(1,96)	1:162:A:GLU:H	1:163:A:ARG:HB3	15	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found